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A detailed static atomistic model has been developed to generate dense, glassy microstructures of bisphenol-A polycarbonate (PC). Microstructures of edge length 18 and 30 Åwere generated using periodic continuation conditions and a potential energy minimization. The analysis of these microstructures has yielded insight into various experimental properties of PC.

The conformation of the individual chains in the bulk were studied, and although analysis of short range structure did not show any strong spacial correlations, there is a tendency for carbonyl bonds to orient parallel at short distances of about 3 Å. No long range was visible due to the small size of the microstructure.

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The distribution of rotation angles in the ensemble of both the 18 and 30 Åmicrostructures indicate that the torsion angles are in some cases widely distributed about their intramolecular minima. This breadth of the distribution highlights the importance of the intermolecular packing.

The elastic constants were calculated by deforming the microstructures by small strain increments of 0.001%. Compression, shear, and tension strains were individually applied to several microstructures and statistical averages of the principal elastic constants were obtained. The calculated values for the shear and bulk moduli are 1520 (± 460) MPa and 6400 (± 2160) MPa, which fall slightly above reported experimental values.

R2

Structure, Relaxation and Physical Aging of Glassy Polymers

SIMULATION OF THE STRUCTURE OF DENSE, AMORPHOUS BISPHENOL-A POLYCARBONATE. Michelle Hutnik, Ali. S. Argon, Massachusetts Institute of Technology, Cambridge, MA; Frank T. Gentile, Peter J. Ludovice, and Ulrich W. Suter, ETH, Zürich, Switzerland.

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A-1